

Libo Li

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72
papers

3,537
citations

27
h-index

59
g-index

73
ext. papers

4,426
ext. citations

5.5
avg, IF

5.87
L-index

#	Paper	IF	Citations
72	MXene molecular sieving membranes for highly efficient gas separation. <i>Nature Communications</i> , 2018 , 9, 155	17.4	530
71	Ethane/ethylene separation in a metal-organic framework with iron-peroxo sites. <i>Science</i> , 2018 , 362, 443-446	33.3	478
70	Effective ion sieving with Ti ₃ C ₂ T _x MXene membranes for production of drinking water from seawater. <i>Nature Sustainability</i> , 2020 , 3, 296-302	22.1	204
69	Water Transport with Ultralow Friction through Partially Exfoliated g-C N Nanosheet Membranes with Self-Supporting Spacers. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 8974-8980	16.4	177
68	The different interactions of lysine and arginine side chains with lipid membranes. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 11906-20	3.4	176
67	Novel inorganic-organic-layered structures: crystallographic understanding of both phase and morphology formations of one-dimensional CdE (E = S, Se, Te) nanorods in ethylenediamine. <i>Inorganic Chemistry</i> , 2003 , 42, 2331-41	5.1	156
66	Paralyzed membrane: Current-driven synthesis of a metal-organic framework with sharpened propene/propane separation. <i>Science Advances</i> , 2018 , 4, eaau1393	14.3	132
65	Water-based routes for synthesis of metal-organic frameworks: A review. <i>Science China Materials</i> , 2020 , 63, 667-685	7.1	103
64	Potential of mean force and pKa profile calculation for a lipid membrane-exposed arginine side chain. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 9574-87	3.4	102
63	Assessing atomistic and coarse-grained force fields for protein-lipid interactions: the formidable challenge of an ionizable side chain in a membrane. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 9588-6023	3.4	99
62	Is arginine charged in a membrane?. <i>Biophysical Journal</i> , 2008 , 94, L11-3	2.9	74
61	Engineering New Defects in MIL-100(Fe) via a Mixed-Ligand Approach To Effect Enhanced Volatile Organic Compound Adsorption Capacity. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 774-782	3.9	69
60	Facile synthesis of hierarchical porous metal-organic frameworks with enhanced catalytic activity. <i>Chemical Engineering Journal</i> , 2018 , 334, 1477-1483	14.7	67
59	Selective gas diffusion in two-dimensional MXene lamellar membranes: insights from molecular dynamics simulations. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 11734-11742	13	61
58	The role of membrane thickness in charged protein-lipid interactions. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012 , 1818, 135-45	3.8	55
57	Ultra-thin titanium carbide (MXene) sheet membranes for high-efficient oil/water emulsions separation. <i>Journal of Membrane Science</i> , 2019 , 592, 117361	9.6	54
56	Simple liquid models with corrected dielectric constants. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 6936-44	3.44	54

55	Recent advances in the synthesis of monolithic metal-organic frameworks. <i>Science China Materials</i> , 2021 , 64, 1305-1319	7.1	51
54	Liquid-Liquid Equilibria for Ternary Systems: Methyl Butyl Ketone + Phenol + Water and Methyl Butyl Ketone + Hydroquinone + Water at 298.15 K and 323.15 K. <i>Journal of Chemical & Engineering Data</i> , 2014 , 59, 2750-2755	2.8	44
53	Atomic Force Microscopy and Molecular Dynamics Simulations for Study of Lignin Solution Self-Assembly Mechanisms in Organic-Aqueous Solvent Mixtures. <i>ChemSusChem</i> , 2020 , 13, 4420-4427	8.3	43
52	Molecular Understanding of the Penetration of Functionalized Gold Nanoparticles into Asymmetric Membranes. <i>Langmuir</i> , 2017 , 33, 361-371	4	38
51	Computer simulations on the pH-sensitive tri-block copolymer containing zwitterionic sulfobetaine as a novel anti-cancer drug carrier. <i>Colloids and Surfaces B: Biointerfaces</i> , 2017 , 152, 260-268	6	37
50	Molecular dynamics simulations of conformation changes of HIV-1 regulatory protein on graphene. <i>Applied Surface Science</i> , 2016 , 377, 324-334	6.7	34
49	Hierarchically structured metal-organic frameworks assembled by hydroxy double salt-Template synergy with high space-time yields. <i>CrystEngComm</i> , 2018 , 20, 1057-1064	3.3	32
48	Protein Translocation through a MoS ₂ Nanopore: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 2070-2080	3.8	32
47	Screening solvents to extract phenol from aqueous solutions by the COSMO-SAC model and extraction process simulation. <i>Fluid Phase Equilibria</i> , 2017 , 451, 12-24	2.5	29
46	Liquid-Liquid equilibria in the ternary systems water + cresols + methyl butyl ketone at 298.2 and 313.2 K: Experimental data and correlation. <i>Fluid Phase Equilibria</i> , 2015 , 404, 89-95	2.5	27
45	Field-SEA: a model for computing the solvation free energies of nonpolar, polar, and charged solutes in water. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 6431-7	3.4	27
44	Liquid-Liquid Equilibria for the Ternary System Mesityl Oxide + Phenol + Water at 298.15, 313.15, and 323.15 K. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 2493-2498	2.8	27
43	Surface Regulation Towards Stimuli-Responsive Luminescence of Ultrasmall Thiolated Gold Nanoparticles for Ratiometric Imaging. <i>Advanced Functional Materials</i> , 2019 , 29, 1806945	15.6	26
42	Phase equilibria of (water + propionic acid or butyric acid + 2-methoxy-2-methylpropane) ternary systems at 298.2 K and 323.2 K. <i>Fluid Phase Equilibria</i> , 2015 , 403, 30-35	2.5	26
41	Simulation insight into the cytochrome c adsorption on graphene and graphene oxide surfaces. <i>Applied Surface Science</i> , 2018 , 428, 825-834	6.7	25
40	Liquid-liquid equilibria for methyl isobutyl ketone + cresols + water at 333.15 K, 343.15 K and 353.15 K: Experimental results and data correlation. <i>Fluid Phase Equilibria</i> , 2016 , 427, 291-296	2.5	25
39	Experimental Determination and Correlation of Liquid-Liquid Equilibria for the Ternary System 2-Methoxy-2-methylpropane + o-Cresol + Water at 298.15 K and 313.15 K. <i>Journal of Chemical & Engineering Data</i> , 2015 , 60, 1396-1400	2.8	24
38	Measurement and thermodynamic modeling of ternary (liquid + liquid) equilibrium for extraction of o-cresol, m-cresol or p-cresol from aqueous solution with 2-pentanone. <i>Journal of Chemical Thermodynamics</i> , 2017 , 104, 230-238	2.9	22

37	Solvent effect on xylose conversion under catalyst-free conditions: insights from molecular dynamics simulation and experiments. <i>Green Chemistry</i> , 2020 , 22, 532-539	10	22
36	Ternary liquid-liquid equilibria for methyl isopropyl ketone-(resorcinol or hydroquinone)-water systems at different temperatures. <i>Fluid Phase Equilibria</i> , 2016 , 429, 93-97	2.5	22
35	Adsorption and separation of propane/propylene on various ZIF-8 polymorphs: Insights from GCMC simulations and the ideal adsorbed solution theory (IAST). <i>Chemical Engineering Journal</i> , 2020 , 386, 1239-1245	14.7	21
34	Determination and modeling of liquid-liquid equilibrium for ternary mixtures of methyl isopropyl ketone, cresol isomers and water. <i>Fluid Phase Equilibria</i> , 2016 , 429, 107-112	2.5	21
33	Understanding the Cellular Uptake of pH-Responsive Zwitterionic Gold Nanoparticles: A Computer Simulation Study. <i>Langmuir</i> , 2017 , 33, 14480-14489	4	20
32	Experimental Determination and Correlation of Liquid-Liquid Equilibria for Methyl Isopropyl Ketone + Phenol + Water Mixtures at 298.15, 313.15, and 323.15 K. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 2221-2225	2.8	18
31	Phase Behavior of an Amphiphilic Block Copolymer in Ionic Liquid: A Dissipative Particle Dynamics Study. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 3998-4005	2.8	17
30	Liquid phase equilibrium of the ternary systems, water + propionic or butyric acid + mesityl oxide, at (298.2 and 323.2) K. <i>Journal of Chemical Thermodynamics</i> , 2017 , 111, 72-79	2.9	15
29	Measurement, correlation and COSMO-SAC prediction of liquid-liquid equilibrium for the ternary systems, mesityl oxide-(o-, m-, p-cresol)-water, at 333.2K and 353.2K. <i>Fluid Phase Equilibria</i> , 2017 , 440, 45-53	2.5	14
28	Measurement and Correlation of Liquid-Liquid Equilibria for the Ternary Methyl Isobutyl Ketone + Phenol + Water System at (333.15, 343.15 and 353.15) K under Atmospheric Pressure. <i>Journal of Solution Chemistry</i> , 2016 , 45, 875-884	1.8	14
27	Computer Simulations on the Channel Membrane Formation by Nonsolvent Induced Phase Separation. <i>Macromolecular Theory and Simulations</i> , 2017 , 26, 1700027	1.5	14
26	Extraction of o-, m- and p-cresol from aqueous solution with methyl isopropyl ketone: Equilibrium, correlations, and COSMO-RS predictions. <i>Journal of Chemical Thermodynamics</i> , 2017 , 115, 180-190	2.9	14
25	Phase Equilibrium for Phenol Extraction from Aqueous Solution with 2-Pentanone at Different Temperatures. <i>Journal of Solution Chemistry</i> , 2016 , 45, 1414-1424	1.8	14
24	Ternary Liquid-Liquid Equilibria for the System 2-Methoxy-2-methylpropane + m-Cresol + Water at 298.15 and 313.15 K: Experimental Data and Correlation. <i>Journal of Solution Chemistry</i> , 2015 , 44, 2393-2404	1.8	13
23	Computer Simulation of DNA Condensation by PAMAM Dendrimer. <i>Macromolecular Theory and Simulations</i> , 2018 , 27, 1700070	1.5	13
22	Measurements and thermodynamic modeling of liquid-liquid equilibria in ternary system 2-methoxy-2-methylpropane+p-cresol+water. <i>Chinese Journal of Chemical Engineering</i> , 2016 , 24, 360-364	2.2	13
21	Liquid-liquid equilibrium for methyl butyl ketone + o-, m-, p-cresol + water ternary systems and COSMO-SAC predictions. <i>Journal of Chemical Thermodynamics</i> , 2018 , 127, 17-24	2.9	13
20	Liquid-liquid equilibrium for ternary systems, methyl isobutyl ketone + (catechol, resorcinol and hydroquinone) + water at 333.15 K, 343.15 K and 353.15 K. <i>Fluid Phase Equilibria</i> , 2017 , 433, 206-211	2.5	11

19	A simple model for growth of semiconductor nanorods using lamellar precursors. <i>Materials Chemistry and Physics</i> , 2005 , 94, 1-6	4.4	9
18	Measurement and correlation of phase equilibrium data of the mixtures consisting of water, resorcinol, mesityl oxide at different temperatures. <i>Chinese Journal of Chemical Engineering</i> , 2018 , 26, 2573-2580	3.2	8
17	Testing the semi-explicit assembly model of aqueous solvation in the SAMPL4 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2014 , 28, 259-64	4.2	8
16	Ternary and Quaternary Liquid-Liquid Equilibria for Systems of Methyl Butyl Ketone + Water + Hydroquinone + Phenol at 313.2 K and Atmospheric Pressure. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 1540-1546	2.8	7
15	Small molecule solvation changes due to the presence of salt are governed by the cost of solvent cavity formation and dispersion. <i>Journal of Chemical Physics</i> , 2014 , 141, 22D518	3.9	7
14	Application of hierarchically porous metal-organic frameworks in heterogeneous catalysis: A review. <i>Science China Materials</i> , 2022 , 65, 298-320	7.1	7
13	Tie-Line Data for Aqueous Mixtures of Butyric Acid with Diisopropyl Ether at Various Temperatures. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 760-765	2.8	6
12	Solvent effect on xylose-to-furfural reaction in biphasic systems: combined experiments with theoretical calculations. <i>Green Chemistry</i> ,	10	6
11	Liquid-Liquid Equilibrium for the Ternary Systems Methyl tert-Butyl Ketone + o-, m-, p-Cresol + Water at (298.2, 313.2, and 323.2) K. <i>Journal of Chemical & Engineering Data</i> , 2017 , 62, 1929-1936	2.8	5
10	Phase Equilibrium Measurement and Thermodynamic Modeling of the 4-Methylpentan-2-one/3-Methylphenol, and 4-Methylphenol/Water Ternary Systems at 298.2, 313.2, and 323.2 K and 0.1 MPa. <i>Journal of Chemical & Engineering Data</i> , 2017 , 62, 141-147	2.8	4
9	Liquid-Liquid Equilibrium of Ternary Systems of Methyl Isobutyl Ketone + o-Cresol + Water at 298.2, 313.2 and 323.2 K. <i>Journal of Solution Chemistry</i> , 2017 , 46, 2204-2213	1.8	4
8	Salt effect on the liquid-liquid equilibrium of the ternary (water + phenol + methyl isobutyl ketone) system: Experimental data and correlation. <i>Chinese Journal of Chemical Engineering</i> , 2019 , 27, 168-173	3.2	4
7	Lysozyme Adsorption on Porous Organic Cages: A Molecular Simulation Study. <i>Langmuir</i> , 2020 , 36, 12299-12308	4	4
6	Identical Composition and Distinct Performance: How ZIF-8 Polymorphs Structures Affect the Adsorption/Separation of Ethane and Ethene. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 3483-3492	2.8	3
5	Chapter 15 Charged Protein Side Chain Movement in Lipid Bilayers Explored with Free Energy Simulation. <i>Current Topics in Membranes</i> , 2008 , 405-459	2.2	2
4	Recent advances in the synthesis of nanoscale hierarchically porous metal-organic frameworks. <i>Nano Materials Science</i> , 2022 ,	10.2	2
3	Molecular dynamics simulation on DNA translocating through MoS ₂ nanopores with various structures. <i>Frontiers of Chemical Science and Engineering</i> , 2021 , 15, 922-934	4.5	2
2	Liquid-Liquid Phase Equilibria for the Ternary Water + Acetic Acid + 3,3-Dimethyl-2-butanone System at (298.15, 313.15 and 323.15) K. <i>Journal of Chemical & Engineering Data</i> , 2015 , 60, 3187-3192	2.8	1

1 Lysozyme Adsorption on Different Functionalized MXenes: A Multiscale Simulation Study. *Langmuir*, 2021, 37, 5932-5942

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